Electro-Thermal-Mechanical Simulation Capability

LLNL has long been a world leader in computational solid mechanics. Recently several solid mechanics codes have become "multiphysics" codes, with the addition of fluid dynamics, heat transfer, and chemistry. However, these multiphysics codes do not incorporate the electromagnetics required for a coupled electro-thermal-mechanical (ETM) simulation. The purpose of this project is to research and develop numerical algorithms for 3-D ETM simulations. There are numerous applications for this capability, such as explosively-driven magnetic flux compressors, electromagnetic launchers, inductive heating and mixing of metals, and MEMS. A robust ETM simulation capability will enable physicists and engineers to better support current DOE programs, and will prepare LLNL for long-term DoD applications.

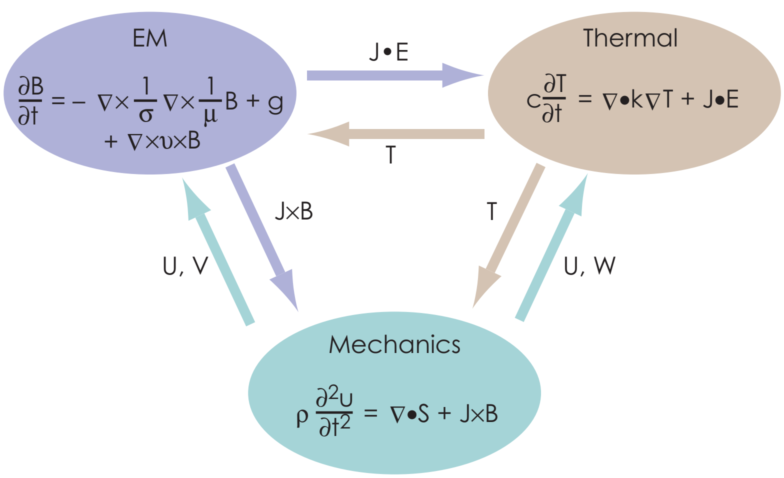

Figure 1. Illustration of the ETM coupling mechanism assumed for this project. The EM module computes the fields *E*, *B* and *J*; the thermal module computes the temperature, *T*; the mechanics module computes the position, *U*, and work, *W*, of the materials.

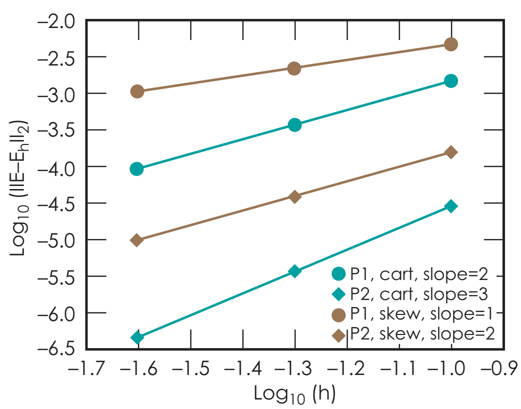

Figure 2. Example convergence result for the higher-order *H(curl)* discretization of the time-dependent eddy current equations. The blue lines are for a Cartesian mesh and show superconvergence; the red lines are for a distorted mesh and illustrate standard $O(h^p)$ convergence.

Project Goals

We define a coupled ETM simulation as a simulation that solves, in a self-consistent manner, the equations of electromagnetics (primarily statics and diffusion), heat transfer (primarily conduction), and nonlinear mechanics (elastic-plastic deformation, and contact with friction). The goal is to add electromagnetics to two existing mechanics codes, ALE3D and Diablo. ALE3D is a heavily used arbitrary-Lagrangian-Eulerian hydrodynamics code; Diablo, currently under development, is an implicit Lagrangian thermal-mechanics code. A finite-element discretization will be used for the electromagnetics. The coupling of the electromagnetic equations, thermal equations, and mechanics equations will be initially done in an operator-split manner. The coupling mechanisms are illustrated in Fig. 1.

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Relevance to LLNL Mission

We are developing a novel simulation capability. With this capability, LLNL will have an unprecedented ability to simulate, design, and optimize ETM systems. This project is aligned with LLNL's core competency in simulation science and engineering. It contributes to the mission to enhance and extend simulation capabilities, and specifically addresses this need in the area of energy manipulation. This project complements ongoing Advanced Simulation and Computing (ASC) work and will use ASC computers and software, such as linear solver packages and visualization tools.

FY2005 Accomplishments and Results

We investigated several different formulations for the electromagnetics, namely the *E*-field formulation, the *H*-field formulation, and the *A-Phi* formulations. We applied the Galerkin procedure to each formulation using *H(curl)*-conforming finite elements, yielding a discrete system of equations that is integrated in time implicitly. The key differences between the three formulations are the *natural* and *essential* boundary conditions. We developed a consistent $O(h^p)$ method for computing the magnetic flux density, *B*, and the induced eddy current density, *J*, for each of the three formulations, and verified the convergence, as shown in Fig. 2.

We have begun to incorporate the electromagnetics into the ALE3D and Diablo codes. In each code the electromagnetics is updated in an operator-split manner, the *JxB* force is added to the momentum equation, and the J*E heating is added to the heat equation. Figure 3 shows the results of a simulation in which a 10-kV capacitor bank is discharged into an aluminum can structure with 1-mm walls. The sequence of images shows the deformation of the can due to the *JxB* force. We will verify this computation with experiments in early FY2006.

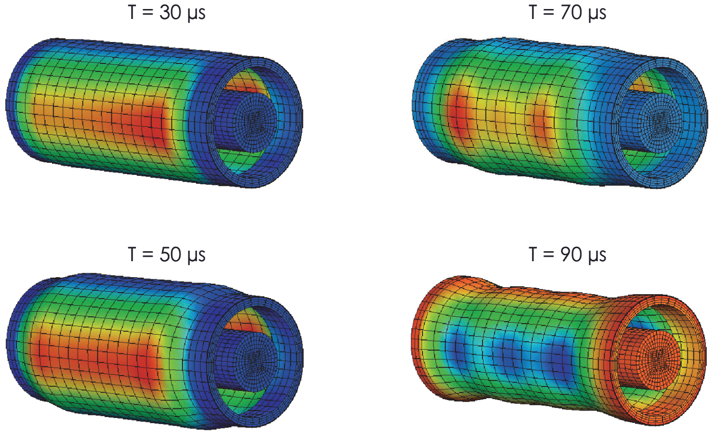

Figure 3. Sequence of snapshots of a preliminary fully-coupled ETM simulation using our EM-enhanced Diablo code. In this experiment a 10-kV capacitor bank is discharged into a can-shaped structure. The color indicates the y-component of the stress caused by the magnetic pressure in the can. The deformation has been exaggerated for clarity.

FY2006 Proposed Work

The following are some of the key research issues that will be investigated during FY2006:

1. Advection of Electromagnetic Quantities. In the ALE3D case, we need the ability to advect electromagnetic fields while still maintaining the divergence-free character of the fields. If the conductivity of the materials is wildly varying, an accurate subzonal interface treatment may be necessary to avoid artificial diffusion of parameters such as current and magnetic flux.
2. Contact/Slide Surfaces. The continuity conditions of electromagnetic fields and currents across material interfaces are somewhat different than for mechanical stress; hence, new algorithms will be developed for contact and slide surfaces.
3. Zero Conductivity Regions. It is not possible to simply set $\sigma = 0$ in the electromagnetic diffusion equation: this would lead to an ill-posed problem. Instead, it is necessary to model air or vacuum regions by some other means. A simple solution is to use small, but nonzero, values of conductivity in air or vacuum regions, and this may be acceptable for many applications. An alternative approach is to solve a magnetostatic problem in the $\sigma = 0$ region, either by finite elements or boundary elements, and this solution must be fully coupled (*i.e.*, solved simultaneously) with the electromagnetic diffusion equation.